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Doping of BN Honeycomb structure: First-Principles Study CAN ATACA, ETHEM AKTURK, SALIM CIRACI — Using first-principles density functional theory calculations, we have investigated the structural, electronic and magnetic properties of monolayer boron-nitride (BN) honeycomb structure which is functionalized by adatom adsorption and by substituting B and N atoms with foreign atom. We considered low and high density coverage of foreign atoms. Generally most of 3d transition metal atoms, some of group 4A, 5A, and 6A elements are bound with significant binding energy and modify the electronic structure of bare BN monolayer resulting in metallic, even half-metallic state. In low coverage case, the bands form by adsorbed atom are flat and charge is mostly localized on the adatom. The band structure of parent BN is not affected except localized states in the band gap.

Can Ataca

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